Analogue Gravity Approach to the Electronic Properties of Curved Graphene

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Abstract

The two-dimensional Dirac material graphene can be bent and folded into countless shapes and structures, in which case the low-energy electronic excitations in the material are described by the mathematics of quantum field theory in curved space and subject to geometric forces analogous to gravity. It is shown how the Dirac equation can be adapted to curved spacetimes using the vierbein picture of general relativity, and this procedure is applied to two different types of 2D systems which can be realised experimentally using graphene: cylindrically symmetric transverse distortions in a place, and a spherical surface. Finally, the relationship between curvature and the emergence of a pseudomagnetic field is discussed.

Acknowledgements

I would like to thank my supervisor, Dr Fabio Biancalana, for his guidance, teaching, and saintly patience over the course of my studies. I would also like to thank the members of the non-linear photonics group for a number of inspiring conversations, and my family for their continued support and encouragement despite my failure to explain to them what I do. Finally, an honourable mention goes to ”et al”, for the enormous number of useful papers they have published under this unusual yet iconic pseudonym.

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Chapter 0

Notation and Convention

0.1 The Metric

Only the spacial dimensions are treated explicitely, and the metric for flat space is taken to be a diagonal matrix whose elements are positive 1.

0.2 Coordinate systems

In order to be as clear as possible, different notation is used to differentiate between coordinates in flat space, curved space, and locally inertial frames. Indices associated with flat space coordinates x^α and the metric $\eta_{\alpha\beta}$ are labelled with the Greek letters $(\alpha, \beta, \gamma ...)$, those associated with coordinates χ^μ defined on a curved manifold with a general Riemannian metric $g_{\mu\nu}$ are labelled with other Greek letters $(\mu, \nu, \rho ...)$, and those associated with a locally defined inertial frame with coordinates ξ^a are labelled with Latin letters $(a, b, c ...)$. Greek indices are used not indicate four spacetime components, nor are Latin indices used to indicate the omission of time as an explicit dimension.

0.3 Summation Convention

Einstein's summation convention is used throughout this thesis. Whenever any term contains a covariant and a contravariant index index with the same label it is to be assumed that this implies a sum over that index.

$$A^{ij}B_{jk} = \sum_j A^{ij}B_{jk} \tag{1}$$

$$X^\mu X^\nu g_{\mu\nu} = \sum_\mu \sum_\nu X^\mu X^\nu g_{\mu\nu} \tag{2}$$

0.4 The Vielbein Field

There is no set convention regarding the ordering of the indices of the vielbein. What some authors refer to as the vielbein, others refer to as the transpose vielbein, and vice versa.

Convention A	Tensor Form	Matrix Form
Covariant	$e_\mu^a e_\nu^b \eta_{ab} = g_{\mu\nu}$	$\mathbf{e}.\eta.\mathbf{e}^{\mathbf{T}} = \mathbf{g}$
Contravariant	$e_a^\mu e_b^\nu g^{ab} = g^{\mu\nu}$	$\mathbf{e}.\eta.\mathbf{e}^{\mathbf{T}} = \mathbf{g}$

Convention B	Tensor Form	Matrix Form
Covariant	$e^a{}_\mu e^b{}_\nu \eta_{ab} = g_{\mu\nu}$	$\mathbf{e}^{\mathbf{T}}.\eta.\mathbf{e} = \mathbf{g}$
Contravariant	$e_a{}^\mu e_b{}^\nu g^{ab} = g^{\mu\nu}$	$\mathbf{e}^{\mathbf{T}}.\eta.\mathbf{e} = \mathbf{g}$

There are no particular trends one way or the other, so I am defining the covariant vielbein to be e_μ^a and the contravariant to be e_a^μ.

Chapter 1

Introduction

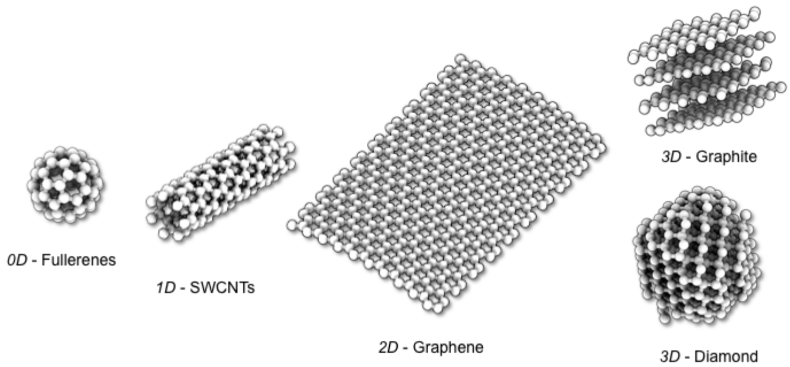


Figure 1.1: Various carbon allotropes
http://graphita.bo.imm.cnr.it/graphita2011/graphene.html

Carbon-based systems show a near-unlimited variety of physical structures and accompanying electronic properties. The two dimensional allotrope graphene, comprised of carbon atoms in a hexagonal “honeycomb” lattice structure, can be seen as the basis for several others. Fullerenes are quasi spheical carbons structures or “graphene balls” that can be described as zero dimensional systems with descrete energy states. Carbon nanotubes are constructed by rolling a layer of graphene and re-attaching the edges, and can be treated as effective one-dimensional systems. Graphite is a three-dimensional material comprised of multiple graphene layers held together by van der Waals forces.

Graphene has achieved celebrity status in recent years as the first truly two dimensional crystal to be discovered and due to demonstrating a variety of remarkable properties, not limited to extraordinary thermal and optical conductivity, strength, and opacity. Central to this thesis is the pseudorelativistic behaviour of graphene’s low energy electronic excitations, which are described by a kind of massless Dirac equation in the two spacial dimensions they are confined to within the graphene monolayer.[1]

Graphene can be bent and folded into any number of shapes including the afforementioned nanotubes and fullerenes. In fact, graphene layers naturally exhibit curvature due to topological defects and rippling. By analogy to the geometric description of gravity emerging from the distortion of spacetime in Einstein's general theory of relativity, the electronic behaviour of graphene in regions of local curvature can be described by a covariant curved-space Dirac equation, and such distortions of the two dimensional layer are felt by the transport electrons as a gravity-like force.[2]

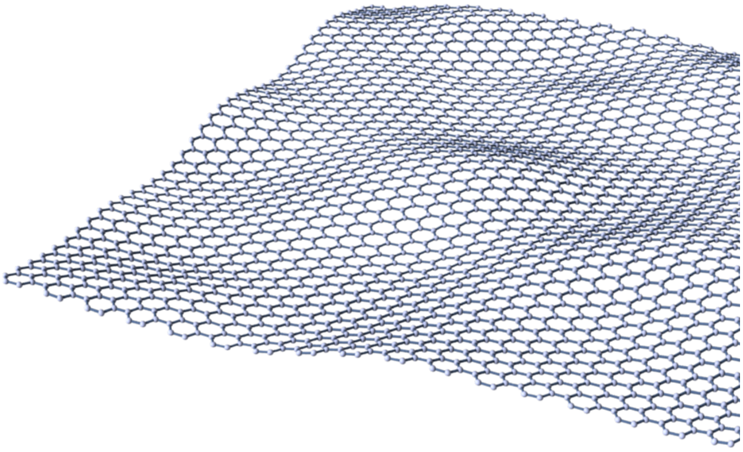


Figure 1.2: A graphene sheet
http://www.jameshedberg.com/scienceGraphics.php?id=graphene-sheet-3D-corner

Quantum theory and general relativity are two of the most central theories in modern physics, and their incompatibility with each other is one of the most famous and widely-debated scientific mysteries of our time. The predictions of both theories have been found to be consistent with experimental observations time and again, quantum theory on a microscopic scale, and general relativity on a cosmological one.

As the two theories operate on completely different scales, experimentation into any sort of middle ground is difficult. It is thought that quantum effects become significant where strong gravitational fields are involved, such as in the viscinity of a black hole or in the early universe, thus a unified theory of quantum gravity may be necessary to understand phenomena in these conditions, but none can be tested since these kinds of fields can't be accessed for experimentation.

Graphene's Dirac-like charge carriers then provide the exciting possibility of measureing the effects of curvature on quantum excitations, which has sparked new interest in the correspondence between such condensed matter systems and quantum field theory in curved space[3][4][5][6][7]. Certain ideal geometries such as a Beltrami pseudosphere[8] can be solved exactly for their theoretical electronic properties using tools like conformal mapping. More generally systems which are not conformally flat must be solved perturbatively for the local density of states[9].

The aim of this thesis is to show how a covariant Dirac theory can be applied to a number of graphene systems to potentially make testable experimental predictions.

Chapter 2

Theory

2.1 Dirac Fermions in Graphene

Graphene is a two-dimensional allotrope of carbon with a hexagonal lattice structure and low-energy electronic excitations which behave like two-dimensional massless Dirac Fermions. These quasiparticles move at the Fermi velocity of graphene, about 300 times smaller than the speed of light, so many of the relativistic effects of quantum electrodynamics show up in graphene but at this much lower speed which is, for our purposes, analogous to the speed of light in this system.

Four of the carbon atom's six electrons are available to form covalent bonds with neighbouring atoms. Three of these form σ-bonds with the three nearest neighbour atoms, forming a trigonal planar structure with a nearest-neighbour separation of 1.42Å. These bonds are responsible for the robustness and flexibility of the lattice, and the trigonal formation leads to the larger hexagonal structure. The remaining p electron forms a much weaker π-bond with one of the nearest neighbours and is free to hop. It is these electrons which are responsible for graphene's electronic properties.

There are two topologically inequivalent sites per unit cell of the hexagonal lattice, comprising two sublattices with different basis vectors, giving rise to a two component spinor wavefunction with each component of the spinor corresponding to a different sublattice.

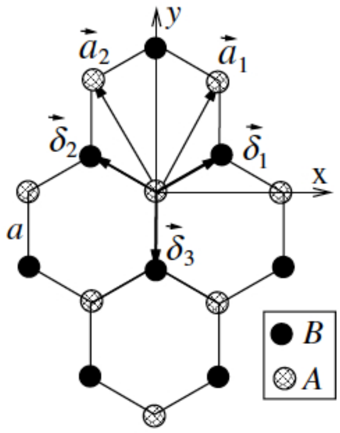


Figure 2.1: Hexagonal structure comprised of two sublattices
Sublattices A and B represented by white and black dots respectively. From Bena et al[10]

The simplest description of the transport electrons in graphene is the nearest neighbour tight-binding model of Wallace[11]. If we assume a finite hopping amplitude $-t$, which is around 2.8eV, then for each wavevector $\mathbf{k}$ the Hamiltonian is

$$\hat{H}(\mathbf{k}) = \begin{pmatrix} 0 & f(\mathbf{k}) \\ f(\mathbf{k}) & 0 \end{pmatrix} \tag{2.1}$$

$$f(\mathbf{k}) = -t \sum_{j=1}^{3} e^{i\mathbf{k}\cdot\delta_j} \tag{2.2}$$

The δ_j are vectors connecting to the nearest neighbours. Hopping only occurs between sublattices A and B, and the on-site energy is taken as the zero of energy, so the diagonal terms are zero.

As a consequence of the sublattice (or chiral) symmetry of this model, the energy spectrum $\varepsilon_\lambda(\mathbf{k}) = \lambda\,|f(\mathbf{k})|$ has a particle-hole symmetry. The band gap closes at two inequivelent points denoted $\mathbf{K}$ and $\mathbf{K}'0$, where $f(\mathbf{K}) = f(\mathbf{K}') = 0$, called “Dirac points”. The theorem of Fermion Doubling guarantees that in 2D lattice models with certain symmetries Dirac points must always appear in pairs. With a single electron per carbon atom free to hop, the negative energy band is full and the positive energy band is empty at zero temperature. Therefore the Fermi energy is zero and the Fermi surface is two isolated points, and the negative and positive energy bands are valence and conduction bands.

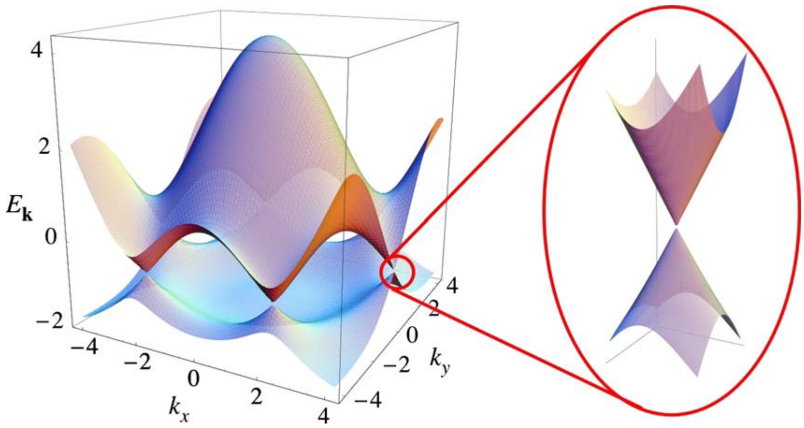


Figure 2.2: Band structure is linear close to Dirac points.
From Castro Neto et al[1]

In the viscinity of the two Fermi points the dispersion is linear, as would be expected in a relativistic theory, rather than quadratic, which is usual for non-relativistic systems. In these regions (low energy or long wavelength excitations with $|\mathbf{q}| \ll |\mathbf{K}|$) we expand the Hamiltonian up to linear order in $\mathbf{q}$, the momentum measured relative to the Dirac point[12][13]

$$\hat{H}(\mathbf{k} = \mathbf{K} + \mathbf{q}) = \tag{2.3}$$

$$\approx \mathbf{q} \cdot \nabla_{\mathbf{k}} \hat{H}|_{\mathbf{K}} \tag{2.4}$$

$$= \hat{H}(\mathbf{q}) \tag{2.5}$$

$$= \frac{3ta}{2} \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} \tag{2.6}$$

$$= \hbar V_f (\sigma \cdot \mathbf{p}) \tag{2.7}$$

This is a massless 2D Dirac Hamiltonian with $V_f = \frac{3ta}{2\hbar}$ playing the role of the speed of light c.

There are three types of spin present in the system. The first is the sublattice pseudospin contained in the two component spinor, the second is the valley isospin associated with the two $\mathbf{K}$, $\mathbf{K}'$ points, and the third is the true spin of the electrons which is not automatically included in 2D Dirac models. In the following we focus on one valley and true spin flavour, as the results are not affected by these spin values.

2.2 The Dirac Equation

The Dirac equation is a relativistic generalisation of the Schrodinger equation. The Schrodinger equation can be obtained by substituting the quantum energy and momentum operators

$$\hat{E} \to i\hbar \frac{\partial}{\partial t} \tag{2.8}$$

$$\hat{p} \to -i\hbar \nabla \tag{2.9}$$

into the classical non-relativistic energy-momentum relation

$$E = \frac{p^2}{2m} + U \tag{2.10}$$

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + U \right) \psi \tag{2.11}$$

Substituting the quantum operators instead into the relativistic relation

$$p_\mu p^\mu = \frac{E^2}{c^2} - p^2 = m^2 c^2 \tag{2.12}$$

yields the Klein-Gordon equation

$$\left(\hbar^2 \partial_\mu \partial^\mu - m^2 c^2 \right) \psi = 0 \tag{2.13}$$

which has plane-wave free particle solutions and succesfully describes the behaviour of scalar quantum fields giving rise to spin-0 particles such as the Higgs Boson. In order to achieve an equation that is first order in time Dirac took the “square root” of the Klein-Gordon operator, in the sense that the Dirac operator multiplies by it’s conjugate to give the Klein-Gordon operator. This was achieved by introducing a set of objects γ, which were found to be matrices, to yield the Dirac equation

$$\left(i\hbar \gamma^\alpha \partial_\alpha - mc \right) \psi = 0 \tag{2.14}$$

Since the electronic excitations in graphene are effectively massless, in this case we are interested in the massless version of the equation

$$i\hbar\gamma^{\alpha}\partial_{\alpha}\psi = 0 \tag{2.15}$$

2.2.1 The Dirac Matrices

There are many possible representations of the Dirac matrices which are equally valid as long as they respect certain conditions. When working in d dimensions, we require d Dirac matrices, each of which is a $n \times n$ square matrix, where n is an even number which is equal to either d or $d-1$. To be consistent with the Klein-Gordon equation it is essential that the the matrices satisfy the anticommutation relation

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu} I_{n\times n} \tag{2.16}$$

For the application to graphene, only two spacial dimensions are required and time is parameterised, so a valid choice (for flat graphene) is

$$\gamma^1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.17}$$

$$\gamma^2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2.18}$$

If a temporal dimension is to be treated explicitely in addition to these two spacial ones, then an extra condition must be imposed. That is

$$(\gamma^0)^{\dagger} = \gamma^0 \tag{2.19}$$

$$(\gamma^j)^{\dagger} = -\gamma^j \tag{2.20}$$

These conditions are satisfied by the following choice

$$\gamma^0 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.21}$$

$$\gamma^1 = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{2.22}$$

$$\gamma^2 = -i\sigma_x = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \tag{2.23}$$

$$\tag{2.24}$$

2.2.2 Solutions and Currents

The Dirac equation described the behaviour of spin-$\frac{1}{2}$ fermions. For a free fermion the wavefunction is the product of a plane wave and a Dirac spinor

$$\psi(x^\alpha) = e^{-ip\cdot x} \begin{pmatrix} u_A(p^\alpha) \\ u_B(p^\alpha) \end{pmatrix} \tag{2.25}$$

$$= e^{-i(\varepsilon t - \mathbf{p}\cdot\mathbf{x})} \begin{pmatrix} u_A(p^\alpha) \\ u_B(p^\alpha) \end{pmatrix} \tag{2.26}$$

The dispersion corresponding to the Dirac Hamiltonian is

$$\varepsilon(\mathbf{k}) = \pm\hbar\sqrt{m_0^2c^2 - c^2\mathbf{k}^2} \tag{2.27}$$

In 2D and 4D, here demonstrate how spinors with the appropriate set of gamma matrices represent a vector with an additional "flag" direction Show the effections of rotations - 2pi rotation of spinor results in same vector with opposite flag

The Fermion current is a space-time vector given by

$$j^\alpha = -eV_f\overline{\psi}\gamma^\alpha\psi \tag{2.28}$$

where $\overline{\psi} = \gamma^0\psi$. The time component, $j^0 = \rho$, is the probability density. The consevation of probability requires that the current satisfies the continuity equation

$$\partial_\alpha j^\alpha = 0 \tag{2.29}$$

2.3 The Dirac Equation in Curved Space

For tensors and tensor fields in curved space we replace the Minkowski metric $\eta_{\alpha\beta}$ with the general Riemannian metric $g_{\mu\nu}$ and the derivative with the covariant derivative.

$$D_\mu A^\nu = \partial_m u A^\nu + \Gamma_{\mu\ \kappa}^{\ \nu} A^\kappa \tag{2.30}$$

While bosons are described by tensor fields, fermions are described by spinor fields, and there is no spinor covariant derivative in terms of the metric, so a different approach is needed in order to describe the electron field in curved space. This approach is the vierbein formalism of general relativity[14].

2.3.1 Non-coordinate Frames

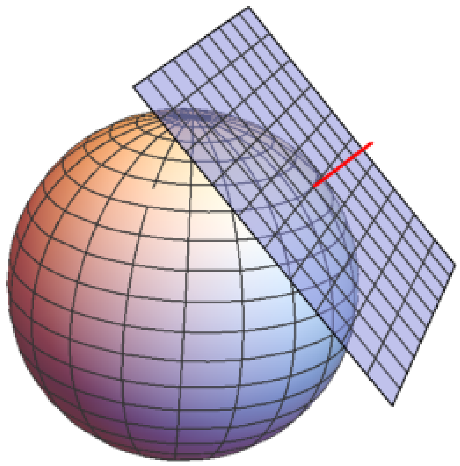


Figure 2.3: Tangent space to a point on a 2-sphere

According to Einstein's principle of equivelence, it is always possible to choose coordinates such that space becomes locally flat. At each point on the manifold with coordinates χ^μ we introduce a locally inertial coordinate system $\xi^a_{\chi_p}(\chi)$, and define the vielbein field

$$e^a_\mu(\chi_p) = \left.\frac{\partial \xi^a_{\chi_p}(\chi)}{\partial \chi^\mu}\right|_{\chi=\chi_p} \tag{2.31}$$

This object is a frame field. It maps each point on the manifold to a set of coordinates in the tangent space to the manifold at that point. That is, the basis vectors of our flat, inertial frame are always tangent to the manifold, so intersect precisely with the coordinate frame at χ. When working in 4D, we call this tetrad or frame field a Vierbein, which is German for ”Four legs”, reffering to the four basis vectors. In three dimensions we have a dreibein, in two a tweibein, in one an einbein. Vielbein means ”many legs” and refers to a frame field in an arbitrary number of dimensions. The coordinate basis is related to the tetrad basis as

$$\hat{e}_\mu(\chi) = e^a_\mu \hat{e}_a(\chi) \tag{2.32}$$

Differentials and derivatives on the manifold can be related to those in the locally flat space

$$e^a_\mu(\chi) d\chi^\mu = d\xi^a \tag{2.33}$$
$$e^\mu_a(\chi) \frac{\partial}{\partial \chi^\mu} = \frac{\partial}{\partial \xi^a} \tag{2.34}$$

The metrics in the two frames are related by

$$g_{\mu\nu}(\chi) = e^a_\mu(\chi) e^b_\nu(\chi) \eta_{ab} \tag{2.35}$$

and the invariant interval is, as ever, invariant.

$$ds^2 = g_{\mu\nu}(\chi) d\chi^\mu d\chi^\nu \tag{2.36}$$
$$= \left[e^a_\mu(\chi) e^b_\nu(\chi) \eta_{ab}\right] d\chi^\mu d\chi^\nu \tag{2.37}$$
$$= \eta_{ab} \left[e^a_\mu(\chi) d\chi^\mu\right] \left[e^b_\nu(\chi) d\chi^\nu\right] \tag{2.38}$$
$$= \eta_{ab} d\xi^a d\xi^b \tag{2.39}$$
$$= ds^2 \tag{2.40}$$

2.3.2 Symmetries of the vierbein field

The vielbein can be thought of as the ”square root” of the metric in a similar way to how the Dirac equation can be thought of as the ”square root” of the Klein-Gordon, and can be considered to be more fundamental. The metric is always necessarily diagonal, while the vielbein is not, so the latter has extra degrees of freedom that are inaccessible to the metric. The vielbein uniquely determines the metric, while the inverse is not true; in squaring the vielbein we lose information which cannot be reconstructed from the metric alone. Two possible vielbeins corresponding to the same matric but different sets of inertial coordinates in the tangent space are related by

$$\bar{e}^a_\mu = e^k_\mu \Lambda^a_k \tag{2.41}$$

Where, in the two dimensional case, Λ^a_k is a one parameter family of transformations encapsulating the extra degree of freedom of the tweibein, but in general is a continuous group of parametric transformations. We require

$$\bar{g}_{\mu\nu} = \bar{e}^a_\mu \bar{e}^b_\nu \eta_{ab} = e^k_\mu \Lambda^a_k e^j_\nu \Lambda^b_j \eta_{ab} = e^k_\mu e^j_\nu (\Lambda^a_k \Lambda^b_j \eta_{ab}) = e^k_\mu e^j_\nu \eta_{kj} = g_{\mu\nu} \tag{2.42}$$

$$\therefore \Lambda \eta \Lambda^T = \eta \tag{2.43}$$

The family of vierbein fields corresponding to the same metric are thus related by the Lorentz transformations, the definition of which is (Eq. 2.43). When the tetrad frame is Lorentz transformed, the metric is unchanged.

Dimension	Independent components		Symmetry
	Vielbein	Metric	
1+1	4	3	β_1
2+0	4	3	σ_3
2+1	9	6	$\beta_1, \beta_2, \sigma_3$
3+0	9	6	$\sigma_1, \sigma_2, \sigma_3$
3+1	16	10	$\beta_1, \beta_2, \beta_3, \sigma_1, \sigma_2, \sigma_3$

2.3.3 Spin Covariant Derivative

With the tweibein, it is possible to express the curved space Dirac equation

$$-i\hbar\hat{\nabla} = -i\hbar\gamma^\mu(\chi)\left(\partial_\mu - \Omega_\mu\right) \tag{2.44}$$
$$= -i\hbar e^\mu_a(\chi)\gamma^a\left(\partial_\mu - \Omega_\mu\right) \tag{2.45}$$
$$= -i\hbar\gamma^a\left(\partial_a - \Omega_a\right) \tag{2.46}$$

The connection Ω_a is a correction to form the "spin covariant derivative". As was stated, there is no general covariant form of the derivative of a spinor in curved space, which is the reason for operating in a field of locally flat frames. To ensure well-behaved transport between the different sets of locally inertial coordinates, quantities in these frames need only transform properly under arbitrary Lorentz transforms

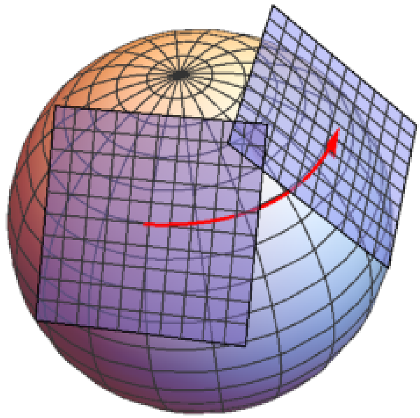


Figure 2.4: Parallel transport of local frames
The spin covariant derivative ensures the proper mapping of quantities from one tangent space to another.

$$\bar{\xi}^a = \Lambda^a_b \xi^b \tag{2.47}$$

$$\bar{\psi}(\bar{\xi}) = S(\Lambda)\,\psi(\xi) = exp\left(-\frac{i}{4}\omega_{ab}\sigma^{ab}\right)\psi(\xi) \tag{2.48}$$

$S(\Lambda)$ is the expansion of the Lorentz transformation Λ in the basis of the spinor-representation generators σ^{ab} which transform the spinor wavefunction ψ[15].

$$\sigma^{ab} = \frac{i}{2}\left[\gamma^a, \gamma^b\right] \tag{2.49}$$

The ω_{ab} are the coefficients of the expansion. The correction Ω_a must be introduced to the derivate to compensate for an extra term that appears in

$$\partial_a \psi(\xi) \rightarrow \bar{\partial}_a \bar{\psi}(\bar{\xi}) = \Lambda^b_a \partial_b \left(S(\Lambda)\,\psi(\xi)\right) \tag{2.50}$$

Expanding Ω in the σ^{ab} basis in the derivative

$$D_a = e^\mu_a \left(\partial_\mu + \Omega_\mu\right) = e^\mu_a \left(\partial_\mu + \frac{i}{2}\omega_{\mu ab}\sigma^{ab}\right) \tag{2.51}$$

$\omega_{\mu ab}$ is the spin connection. Its role in the tangent space is analogous to that of the affine connect $\Gamma^{\kappa}_{\mu\,\nu}$ on the manifold, in that

$$D_\mu X^\nu = \partial_\mu X^\nu + \Gamma^{\ \nu}_{\mu\ \kappa} X^\kappa \tag{2.52}$$

$$D_\mu X^a = \partial_\mu X^a + \omega_{\mu\ b}^{\ a} X^b \tag{2.53}$$

It can be determined by demanding that the two pictures are consistent[14]

$$D_\mu X^a = \partial_\mu X^a + \omega_{\mu\ b}^{\ a} X^b \tag{2.54}$$

$$= \partial_\mu \left(e^{\ a}_\nu X^\nu\right) + \omega_{\mu\ b}^{\ a} \left(e^{b}_{\ \nu} X^\nu\right) \tag{2.55}$$

$$= \partial_\mu X^\nu + \Gamma^{\ \kappa}_{\mu\ \nu} X^\kappa \tag{2.56}$$

$$\omega_{\mu\ b}^{\ a} = e^{\ a}_\nu e^\lambda_b \Gamma^{\ \nu}_{\mu\ \lambda} - e^\lambda_b \partial_\mu e^a_\lambda \tag{2.57}$$

2.3.4 Dirac Currents in Curved Space

The Dirac currents are given in terms of the curved space matrices and solutions to the covariant Dirac equation by

$$j^\mu = -eV_f \overline{\psi} \gamma^\mu \psi \tag{2.58}$$

and the continuity equation becomes

$$D_\mu j^\mu = \tag{2.59}$$

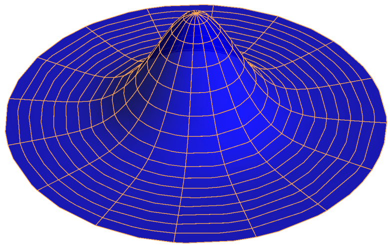
$$\partial_\mu j^\mu + \Gamma^{\ \mu}_{\mu\ \nu} j^\nu = \tag{2.60}$$

$$\frac{1}{\sqrt{|g|}} \partial_\mu \left(\sqrt{|g|} j^\mu\right) = 0 \tag{2.61}$$

where g is the determinant of the metric.

Chapter 3

Transverse Distortions



Out of plane deformations in an otherwise flat graphene sheet can occur due to defects, but more significantly mechanical oscillations are to be expected at any reasonable temperature. Fluxuron modes manifest as out-of-plane oscillations like this manifold. The mechanical crystal vibration is slow enough compared to the motion of electrons through the material that the manifold they live on is bumpy but effectively stationary. In this Chapter we focus on curvature due to out-of-plane deformations with cylindrical symmetry, beginning with the Dirac equation in polar coordinates.

3.1 Dirac equation in polar coordinates

Even in the absense of physical curvature, the behaviour of polar coordinate systems shows some aspects of a curved system. We can express the covariant Dirac equation in polar coordinates using the tweibein and spin connection. The metric in plane polar coordinates is

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix} \tag{3.1}$$

$$\tag{3.2}$$

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{r^2} \end{pmatrix} \tag{3.3}$$

The tweibein field which acts as the transformation between this space and the tangent space with the local metric $diag(1,1)$ can in general be found from a Cholesky decomposition of $g_{\mu\nu}$ or $g^{\mu\nu}$, or from an LDL decomposition should time be included in the metric, making it non positive definite. In this case, since the metric is diagonal an obvious candidate for the tweibein presents itself easily

$$e^a_\mu = \begin{pmatrix} 1 & 0 \\ 0 & r \end{pmatrix} \tag{3.4}$$

$$e^\mu_a = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{r} \end{pmatrix} \tag{3.5}$$

This is called the "natural", "diagonal" or "rotating" tweibein. In this case, the curved γ-matrices are

$$\gamma^r(\chi) = \gamma^1 \tag{3.6}$$

$$\gamma^\theta(\chi) = \frac{1}{r}\gamma^2 \tag{3.7}$$

$$\tag{3.8}$$

the nonzero components of the affine connection are

$$\Gamma^r_{r\,\theta} = -r^2 \tag{3.9}$$

$$\Gamma^r_{\theta\,\theta} = \Gamma^\theta_{r\,\theta} = \frac{1}{r} \tag{3.10}$$

$$\tag{3.11}$$

and the nonzero components of the spin connection are

$$\omega_{\theta\,2}^{1} = -\omega_{\theta\,1}^{2} = 1 \tag{3.12}$$

The covariant Dirac equation in polar coordinates is

$$\begin{pmatrix} i\partial_t & \partial_r + \frac{1}{2r} + \frac{i}{r}\partial_\theta \\ -\partial_r - \frac{1}{2r} + \frac{i}{r}\partial_\theta & -i\partial_t \end{pmatrix} \psi(t,r,\theta) = 0 \tag{3.13}$$

Alternatively we could choose the tweibein with a rotation by θ to express the new γ^μ as projections of the fixed matrices in cylindrical coordinates, called the "fixed" or "Cartesian" tweibein[16][17]. Our local matrices in the "rotating" frame are then related to these by a transformation

$$S(\theta) = e^{i\sigma_3 \frac{\theta}{2}} \tag{3.14}$$

$$\gamma^{\mu}{}_{rot} = S\gamma^{\mu}{}_{cart} S^{-1} \tag{3.15}$$

In this fixed coordinate system there are no spin connections and the Hamiltonian is

$$\hat{H}_{cart} = \begin{pmatrix} 0 & e^{-i\theta}\left(\partial_r - \frac{i}{r}\partial_\theta\right) \\ e^{i\theta}\left(\partial_r + \frac{i}{r}\partial_\theta\right) & 0 \end{pmatrix} \tag{3.16}$$

The Hamiltonian in the diagonal or rotating gauge, representing a local frame where the γ^μ matrices are independent of θ is related to this Hamiltonian by

$$H_{rot} = SH_{cart}S^{-1} \tag{3.17}$$

$$= \begin{pmatrix} 0 & e^{i\frac{\theta}{2}} e^{-i\theta}\left(\partial_r - \frac{i}{r}\partial_\theta\right) e^{i\frac{\theta}{2}} \\ e^{-i\frac{\theta}{2}} e^{i\theta}\left(\partial_r + \frac{i}{r}\partial_\theta\right) e^{-i\frac{\theta}{2}} & 0 \end{pmatrix} \tag{3.18}$$

$$= \begin{pmatrix} 0 & \partial_r + \frac{1}{2r} - \frac{i}{r}\partial_\theta \\ \partial_r + \frac{1}{2r} + \frac{i}{r}\partial_\theta & 0 \end{pmatrix} \tag{3.19}$$

$$\tag{3.20}$$

and the wavefunction solutions in these two frames are related by

$$\psi_{rot} = S\psi_{cart} \tag{3.21}$$

3.1.1 Eigeinstates

The advantage of the local rotating frame is that the γ^{μ} are independent of θ so we use a simple separation of variables to solve the equation.

$$\psi_{km\lambda}(t,r,\theta) = R_{km\lambda}(r)\,\Theta_m(\theta)\,e^{-i\varepsilon_k t} \tag{3.22}$$

$$R_{km\lambda}(r) = \sqrt{\frac{k}{\sqrt{2}}}\begin{pmatrix} J_m(kr) \\ i\lambda J_{(m+1)}(kr) \end{pmatrix} \tag{3.23}$$

$$\Theta_m(\theta) = e^{i\left(m+\frac{1}{2}\right)\theta} \tag{3.24}$$

Where J_m is the Bessel function of order m.

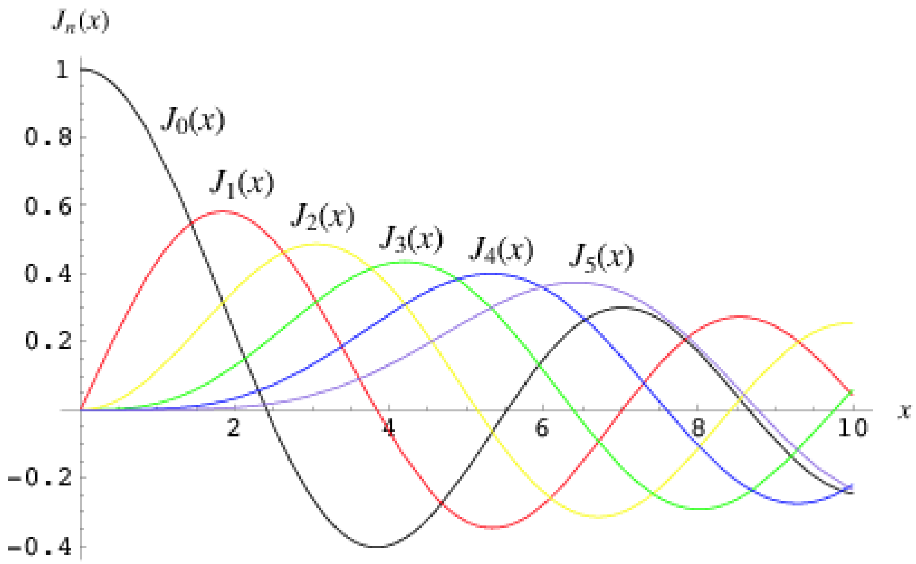


Figure 3.1: Bessel functions of orders 0 to 5
Image from http://mathworld.wolfram.com/BesselFunctionoftheFirstKind.html

So the complete eigenstates are

$$\psi_{km\lambda}(t,r,\theta) = \sqrt{\frac{k}{\sqrt{2}}}e^{-i\varepsilon_k t}e^{i\left(m+\frac{1}{2}\right)\theta}\begin{pmatrix} J_m(kr) \\ i\lambda J_{(m+1)}(kr) \end{pmatrix} \tag{3.25}$$

The energies ε_k are the well known continuous energy spectrum of graphene

$$\varepsilon_{k,\lambda} = \lambda\hbar v_f|k| \tag{3.26}$$

$\lambda = \pm 1$ labels particle and hole states respectively, and m is an integer so that the angular part $e^{i\left(m+\frac{1}{2}\right)\theta}$ satisfies the condition

$$\psi(\theta+2\pi) = -\psi(\theta) \tag{3.27}$$

for a spinor under local rotations. The solutions in the fixed coordinates[18]

$$\psi_{km\lambda}(t,r,\theta) = \sqrt{\frac{k}{\sqrt{2}}}e^{-i\varepsilon t}\begin{pmatrix} e^{im\theta}J_m(kr) \\ i\lambda e^{i(m+1)\theta}J_{(m+1)}(kr) \end{pmatrix} \tag{3.28}$$

behave instead as

$$\psi(\theta+2\pi) = \psi(\theta) \tag{3.29}$$

because in this case a change in θ corresponds to an external rotation with respect to a fixed coordinate system, rather than an internal rotation. In both cases the angular momentum eigenvalues are $\left(m+\frac{1}{2}\right)\hbar$

$$\begin{aligned}
\hat{L}_{z,rot} &= S\hat{L}_{z,cart}S^{-1} && (3.30)\\
&= -i\hbar\partial\theta && (3.31)\\
\hat{L}_{z,cart} &= -i\hbar\partial\theta + \frac{\hbar}{2}\sigma_z && (3.32)\\
\hat{L}_{z,rot}\psi_{rot} &= \left(m+\frac{1}{2}\right)\hbar\psi_{rot} && (3.33)\\
\hat{L}_{z,cart}\psi_{cart} &= \left(m+\frac{1}{2}\right)\hbar\psi_{cart} && (3.34)
\end{aligned}$$

3.1.2 Plane wave soltutions

The physical free solutions to the Dirac equation and the flat graphene Hamiltonian are known to be plane waves. The orthonormal eigenstates ψ_{km} we have found correspond to a single component of a partial-wave expansion of the physical free solutions. Using the partial wave expansion for a scalar plane wave in terms of Bessel functions

$$e^{i\underline{\mathrm{k}}\cdot\underline{\mathrm{r}}} = \sum_{m=-\infty}^{\infty} i^m e^{-im\theta_k}\left[J_m(kr)\,e^{im\theta}\right] \tag{3.35}$$

We are able to express a spinor plane wave in a similar way

$$\frac{1}{\sqrt{2}}e^{i\underline{\mathrm{k}}\cdot\underline{\mathrm{r}}}\begin{pmatrix}1\\ \lambda e^{i\theta_k}\end{pmatrix}=\sum_{m=-\infty}^{\infty}\frac{i^m}{\sqrt{k}}e^{-im\theta_k}\left[\sqrt{\frac{k}{\sqrt{2}}}\begin{pmatrix}e^{im\theta}J_m(kr)\\ i\lambda e^{i(m+1)\theta}J_{(m+1)}(kr)\end{pmatrix}\right] \tag{3.36}$$

$$=\sqrt{\frac{1}{\sqrt{2}}}\begin{pmatrix}\sum_{m=-\infty}^{\infty}i^m e^{-im\theta_k}\left[e^{im\theta}J_m(kr)\right]\\ \sum_{m+1=-\infty}^{\infty}i^{m+1}e^{-i(m+1)\theta_k}\left[e^{i(m+1)\theta}J_{(m+1)}(kr)\right]e^{i\theta_k}\end{pmatrix} \tag{3.37}$$

$$\tag{3.38}$$

3.1.3 Dirac Currents in Polar Coordinates

The current operator j^μ in terms of the new γ^μ in this coordinate system is

$$j^\mu=-ev_f\left(\mathbf{I},\sigma^x,\frac{1}{r}\sigma^y\right) \tag{3.39}$$

and the continuity equation is

$$\frac{1}{\sqrt{|g|}}\partial_\mu\left(\sqrt{|g|}j^\mu\right)=\frac{1}{r}\partial_\mu\left(r\cdot j^\mu\right)\qquad=0 \tag{3.40}$$

3.2 Graphene with a bump

We can introduce cylindrically symmetrical out of plane deformations first as a constrained z-coordinate as a function of r in the lab frame

$$x=r\cos(\theta) \tag{3.41}$$

$$y=r\sin(\theta) \tag{3.42}$$

$$z=f(r) \tag{3.43}$$

We can write the invariant interval on the surface as

$$dS^2 = dr^2 + r^2 d\theta^2 + dz^2 \tag{3.44}$$

$$= dr^2 + r^2 d\theta^2 + \left(\frac{df(r)}{dr}\right)^2 dr^2 \tag{3.45}$$

$$= \left(1 + \left(\frac{df(r)}{dr}\right)^2\right) dr^2 + r^2 d\theta^2 \tag{3.46}$$

and the metric in the 2D surface frame is then

$$g_{\mu\nu} = \begin{pmatrix} 1+f'^2 & 0 \\ 0 & r^2 \end{pmatrix} \tag{3.47}$$

$$\tag{3.48}$$

$$g^{\mu\nu} = \begin{pmatrix} \frac{1}{1+f'^2} & 0 \\ 0 & \frac{1}{r^2} \end{pmatrix} \tag{3.49}$$

The tweibein is

$$e^{\,a}_{\mu} = \begin{pmatrix} \sqrt{1+f'^2} & 0 \\ 0 & r \end{pmatrix} \tag{3.50}$$

$$e^{\mu}_{\,a} = \begin{pmatrix} \frac{1}{\sqrt{1+f'^2}} & 0 \\ 0 & \frac{1}{r} \end{pmatrix} \tag{3.51}$$

the nonzero components of the affine connection are

$$\Gamma^{r}_{r\,r} = \frac{f' f''}{1+f'^2} \tag{3.52}$$

$$\Gamma^{r}_{r\,\theta} = \frac{-r^2}{1+f'^2} \tag{3.53}$$

$$\Gamma^{r}_{\theta\,\theta} = \Gamma^{\theta}_{r\,\theta} = \frac{1}{r} \tag{3.54}$$

$$\tag{3.55}$$

and the nonzero components of the spin connection are

$$\omega_{\theta}{}^{1}{}_{2} = -\omega_{\theta}{}^{2}{}_{1} = \frac{1}{\sqrt{1+f'^2}} \tag{3.56}$$

The curved space γ-matrices become

$$\gamma^r(\chi) = \frac{1}{\sqrt{1+f'^2}}\gamma^1 \tag{3.57}$$

$$\gamma^\theta(\chi) = \frac{1}{r}\gamma^2 \tag{3.58}$$

If we choose again $\gamma^a = (-i\sigma_y, i\sigma_x)$, the curved space Dirac equation $-i\gamma^\mu(\mathbf{x}')D_\mu\psi = 0$ is

$$\begin{pmatrix} i\partial_t & \frac{1}{\sqrt{1+f'^2}}\left(\partial_r + \frac{1}{2r}\right) + \frac{i}{r}\partial_\theta \\ -\frac{1}{\sqrt{1+f'^2}}\left(\partial_r + \frac{1}{2r}\right) + \frac{i}{r}\partial_\theta & -i\partial_t \end{pmatrix} \psi(t,r,\theta) = 0 \tag{3.59}$$

The current operator and continuity equation also change with the introduction of this distortion

$$j^\mu = -ev_f\left(\mathbf{I}, \frac{1}{\sqrt{1+f'(r)^2}}\sigma^x, \frac{1}{r}\sigma^y\right) \tag{3.60}$$

$$\frac{1}{r\sqrt{1+f'(r)^2}}\partial_\mu\left(r\sqrt{1+f'(r)^2}\cdot j^\mu\right) = 0 \tag{3.61}$$

3.2.1 Perturbation theory

In general this system can only be solved by considering the deformation to be a perturbation to the exactly solvable case of flat graphene, as the metric is not conformally flat. We can express the Hamiltonian in the curved space as a correction to the flat Hamiltonian to first order in a small parameter α as

$$H_{rot} = -i\hbar v_f \begin{pmatrix} 0 & \partial_r + \frac{1}{2r} - \frac{i}{r}\partial_\theta \\ \partial_r + \frac{1}{2r} + \frac{i}{r}\partial_\theta & 0 \end{pmatrix} \tag{3.62}$$

$$+\frac{i}{2}\alpha\hbar v_f f'^2 sin^2(\omega t)\begin{pmatrix} 0 & \partial_r + \frac{1}{2r} \\ \partial_r + \frac{1}{2r} & 0 \end{pmatrix} \tag{3.63}$$

$$\tag{3.64}$$

It will not do to apply standard perturbation theory to find global transitions between states induced by the perturbation Hamiltonian. The effect of the curvature is to induce a local density of states which varies with r, which in studies of systems of this kind such as[9] and[19] is found by calculating the Green's function of the interaction Hamiltonian. The local density of states is then

$$\rho(r) = -\frac{1}{\pi} Im\left[G(r,r)\right] \tag{3.65}$$

3.2.2 Mechanical Oscillations

In many cases, the distortion of the graphene sheet will not be constant but periodic in time. The characteristic speed of mechanical motion in the graphene sheet will be much smaller than the Fermi velocity, so time does not need to be treated explicitely.

To extend the above case to one in which the deformation oscillates with a single angular frequency ω we include time t as a parameter in the surface function

$$\begin{aligned} f(r) \to & f(r,t) && (3.66)\\ =& f(r)\sin(\omega t) && (3.67) \end{aligned}$$

We can go further and add more oscillatory transverse distortions by defining the constrained $z(r)$ as

$$\begin{aligned} z =& F(r) && (3.68)\\ =& \sum_j f_j(r)\sin\left(\omega_j t\right) && (3.69) \end{aligned}$$

As t is a parameter, the only effect this has on the behaviour of the system is to replace all instances of $f'(r)^2$ with $F'(r)^2 = \sum_j f_j'(r)^2 \sin^2\left(\omega_j t\right)$. When solving perturbatively to first order in the small parameter, this increases the number of terms in the interaction potential but doesn't change the complexity of the problem.

$$\begin{aligned} H_{rot} = & -i\hbar v_f \begin{pmatrix} 0 & \partial_r + \frac{1}{2r} - \frac{i}{r}\partial_\theta \\ \partial_r + \frac{1}{2r} + \frac{i}{r}\partial_\theta & 0 \end{pmatrix} && (3.70)\\ & + \frac{i}{2}\alpha\hbar v_f \sum_j \left(f_j'(r)^2 \sin^2\left(\omega_j t\right)\right) \begin{pmatrix} 0 & \partial_r + \frac{1}{2r} \\ \partial_r + \frac{1}{2r} & 0 \end{pmatrix} && (3.71) \end{aligned}$$

Chapter 4

Graphene 2-Sphere

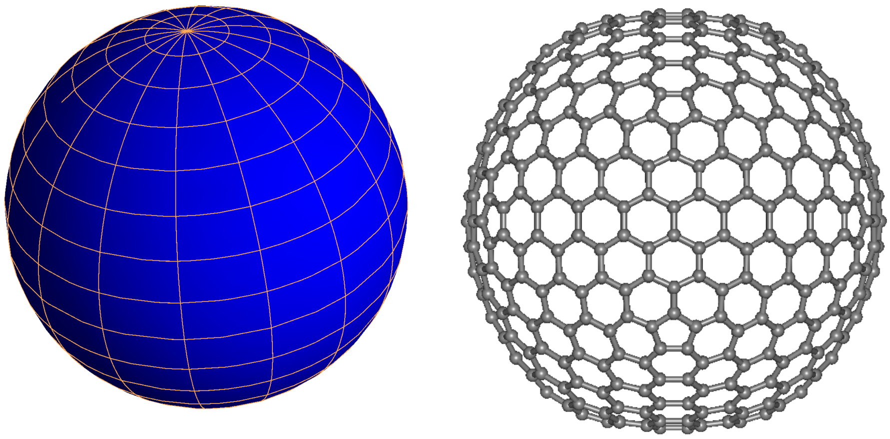


Figure 4.1: Left: 2-sphere geomtry. Right: C_{540} molecule
Fullerene image from http://www.nanotube.msu.edu/fullerene/fullerene-isomers.html

The 2-sphere is a simple but interesting case. A free massless Dirac field on a 2-sphere closely resembles many fullerenes - large hollow spheroidal molecules made up of many carbon atoms, often in an approximately hexagonal lattice, resembling ”balls of graphene”. The most famous example is the Buckminsterfullerine or ”Buckyball”, made up of 60 carbon atoms arranged in the shape of a football. Another, made up of 540 carbon atoms, is depicted in (Fig. 4.1).

4.1 Dirac Equation on the Sphere

To construct the Dirac equation on the surface of the sphere, we again begin from the metric to construct new γ-matrices and a spin connection. The metric on the sphere in terms of the coordinate $\chi = \chi(\theta, \phi)$ is

$$g_{\mu\nu} = \begin{pmatrix} r^2 & 0 \\ 0 & r^2\sin^2(\theta) \end{pmatrix} \tag{4.1}$$

$$\tag{4.2}$$

$$g^{\mu\nu} = \left(g_{\mu\nu}\right)^{-1} \tag{4.3}$$

$$= \begin{pmatrix} \frac{1}{r^2} & 0 \\ 0 & \frac{1}{r^2\sin^2(\theta)} \end{pmatrix} \tag{4.4}$$

As the metric is diagonal, we can easily see that the natural tweibein is

$$e_{\mu}^{a} = \begin{pmatrix} r & 0 \\ 0 & r\sin(\theta) \end{pmatrix} \tag{4.5}$$

$$e_{a}^{\mu} = \begin{pmatrix} \frac{1}{r} & 0 \\ 0 & \frac{1}{r\sin(\theta)} \end{pmatrix} \tag{4.6}$$

The affine connection on the 2-sphere is

$$\Gamma^{\kappa}_{\mu\,\nu} = \frac{1}{2} g^{\kappa\rho}\left(\partial_\mu g_{\nu\rho} + \partial_\nu g_{\mu\rho} - \partial_\rho g_{\mu\nu}\right) \tag{4.7}$$

$$= \begin{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ -\cos(\theta)\sin(\theta) \end{pmatrix} \\ \begin{pmatrix} 0 \\ \cot(\theta) \end{pmatrix} & \begin{pmatrix} \cot(\theta) \\ 0 \end{pmatrix} \end{pmatrix} \tag{4.8}$$

and the spin connection is

$$\omega_{\mu\,b}^{\,a} = e_{\nu}^{a} e_{\nu}^{\lambda} \Gamma^{\nu}_{\mu\,\lambda} - e_{b}^{\lambda}\partial_\mu e_{\lambda}^{a} \tag{4.9}$$

$$= \begin{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 \\ -\cos(\theta) \end{pmatrix} & \begin{pmatrix} \cos(\theta) \\ 0 \end{pmatrix} \end{pmatrix} \tag{4.10}$$

However we choose to define the flat space Dirac matrices γ^1 and γ^2, the Dirac matrices on the sphere are then

$$\gamma^{\mu}(\chi) = e^{\mu}_{a}(\chi)\gamma^{a} \tag{4.11}$$

$$\gamma^{\theta}(\chi) = \frac{1}{r}\gamma^{1} \tag{4.12}$$

$$\gamma^{\phi}(\chi) = \frac{1}{r\sin(\theta)}\gamma^{2} \tag{4.13}$$

The spin covariant derivative is

$$\Omega_{\mu} = \frac{1}{8}\omega_{\mu ab}\Sigma^{ab} \tag{4.14}$$

where Σ^{ab} is the antisymmetric tensor formed by the commutator $[\gamma^{a},\gamma^{b}]$. If we define the flat dirac matrices to be

$$\gamma^{1} = \sigma_{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4.15}$$

$$\gamma^{2} = \sigma_{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{4.16}$$

The curved space Dirac equation $-i\gamma^{\mu}(\chi)D_{\mu}\psi = 0$ then becomes

$$\begin{aligned}
-i\gamma^{\mu}(\chi)D_{\mu}\psi &= i\left[\gamma^{\theta}(\chi)\left(\partial_{\theta}+\Omega_{\theta}\right)+\gamma^{\phi}(\chi)\left(\partial_{\phi}+\Omega_{\phi}\right)\right]\psi && (4.17)\\
&= -i\left[\frac{1}{r}\sigma_{x}\partial_{\theta}+\frac{1}{r\sin(\theta)}\sigma_{y}\left(\partial_{\phi}-\frac{i\sigma_{z}}{2}\cos(\theta)\right)\right]\psi && (4.18)\\
&= -i\left[\frac{1}{r}\sigma_{x}\left(\partial_{\theta}+\frac{\cot(\theta)}{2}\right)+\frac{1}{r\sin(\theta)}\sigma_{y}\partial_{\phi}\right]\psi = 0 && (4.19)
\end{aligned}$$

The current operator is

$$\begin{aligned}
j^{\mu} &= -ev_{f}\gamma^{0}\gamma^{\mu} && (4.20)\\
&= -ev_{f}\left(\mathbf{I},\frac{1}{r}\sigma^{x},\frac{1}{r\sin(\theta)}\sigma^{y}\right) && (4.21)
\end{aligned}$$

and the continuity condition is

$$D_\mu j^\mu = \tag{4.22}$$

$$\frac{1}{\sqrt{|g|}}\partial_\mu\left(\sqrt{|g|}j^\mu\right) \tag{4.23}$$

$$\frac{1}{r\sin(\theta)}\partial_\mu\left(r\sin(\theta)\cdot j^\mu\right) = 0 \tag{4.24}$$

4.1.1 Solutions to the Dirac Equation on the 2-sphere

The topology of the 2-sphere is fundamentally different to that of a 2D plane. Unlike the case of a layer with transverse distortions considered in the previous chapter, particles confined to the spherical surface can no longer be considered to be free and the energy levels are quantised.

The solutions to the Dirac operator on this space are found by a lengthy process in[20] [21]. The eigenvalues are the positive integers

$$\lambda = \frac{\hbar c}{r}\left(n + |m| + \frac{1}{2}\right) \tag{4.25}$$

$$n = 1, 2, 3... \tag{4.26}$$

$$m = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}... \tag{4.27}$$

where m is the projection of the angular momentum in units of $\hbar$ as usual. The 2-sphere has a closed topology in addition to its constant curvature, so the energies are discrete. The eigenstates are a complete orthonormal set of spinor functions called the spinor spherical functions. These are shown in (Fig. 4.2) and written as

$$\Upsilon^{\pm}_{lm}(x,\phi) = \pm\frac{i^{l^+}(-1)^{l^-}}{2^{l^+}\Gamma(l^+)}\sqrt{\frac{(l+m)!}{(l-m)!}} \tag{4.28}$$

$$\times\frac{e^{im\phi}}{\sqrt{2\pi}}\begin{pmatrix}\sqrt{\mp i}\,(1-x)^{-\frac{m^-}{2}}(1+x)^{-\frac{m^+}{2}}\frac{\partial^{l-m}}{\partial x^{l-m}}(1-x)^{l^-}(1+x)^{l^+}\\ \sqrt{\pm i}\,(1-x)^{-\frac{m^+}{2}}(1+x)^{-\frac{m^-}{2}}\frac{\partial^{l-m}}{\partial x^{l-m}}(1-x)^{l^+}(1+x)^{l^-}\end{pmatrix} \tag{4.29}$$

where

$$x = cos(\theta) \tag{4.30}$$

$$l^{\pm} = l \pm \frac{1}{2} \tag{4.31}$$

$$m^{\pm} = m \pm \frac{1}{2} \tag{4.32}$$

$$\Gamma(n) = (n-1)! \tag{4.33}$$

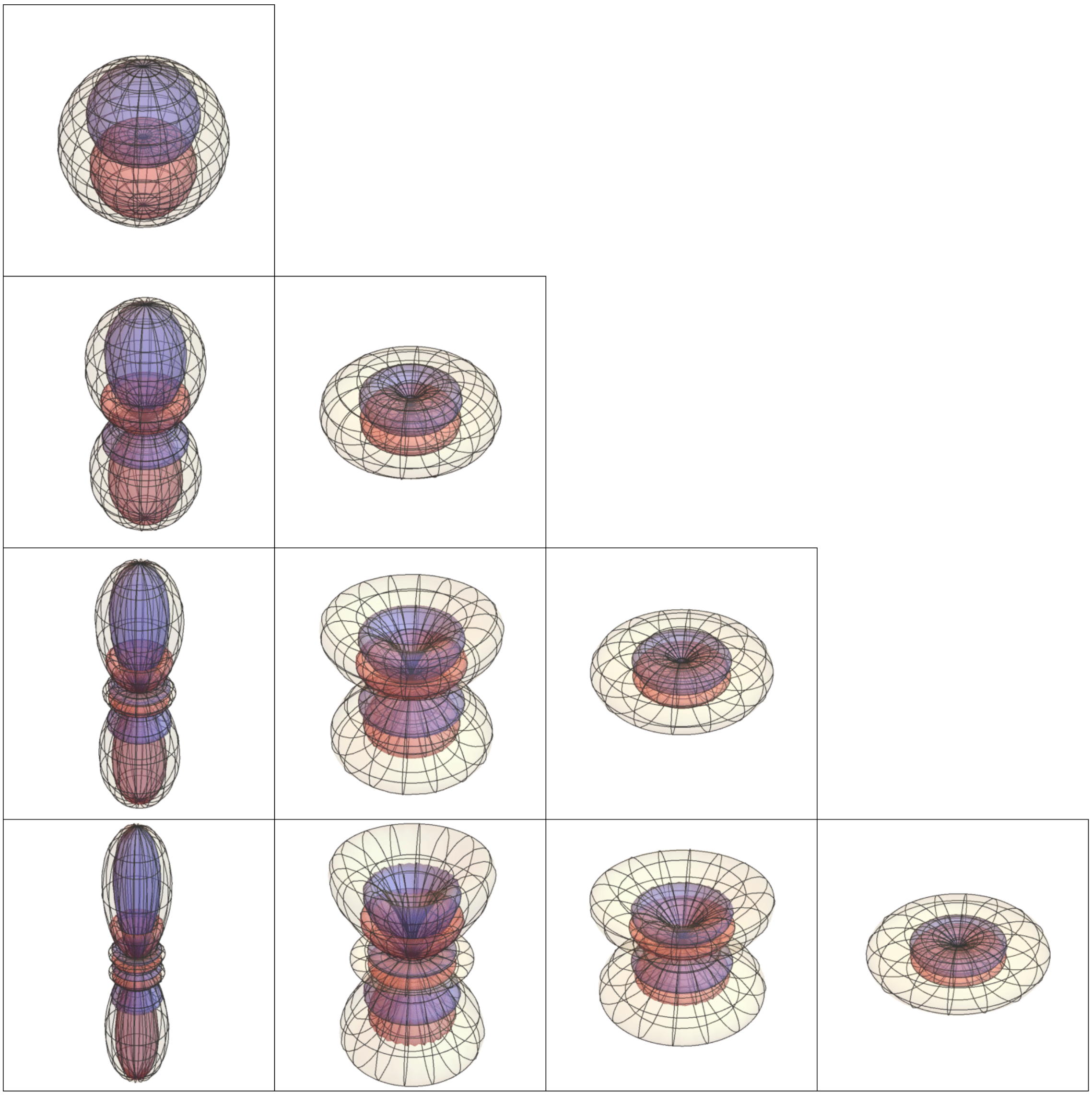


Figure 4.2: Spinor Spherical Harmonics
The first spinor spherical harmonics with $j = l + s$, $s = \frac{1}{2}$ and $m > 0$. From top to bottom $l = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ and from left to right $m = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$. Blue and red respectively represent the upper and lower components of the spinor, and white represents the total probability density of the state

The spinor spherical functions are different but related to conventional spherical spinors $\Omega_{j,l,m}$, which are found in spherical coordinates in flat 3D space rather than the curved space of the S^2 manifold. The $\Omega_{j,l,m}$ comprise a different orthonormal representation on the sphere so when the spinor spherical functions Υ are transform to a description in Cartesian coordinates, they can be expressed as combinations of the $\Omega_{j,l,m}$ with the same total angular momentum j and z-projection of the total angular momentum m .

Chapter 5

Curvature as a Pseudomagnetic Field

5.1 Relation in 2D

Here it is proved that a Dirac field existing on a 2-manifold with a diagonal metric experiences gravitational effects as an effective magnetic field whose magnitude is everywhere proportional to the scalar curvature by a given factor and whose direction is everywhere normal to the manifold.

5.1.1 The general form of the Ricci scalar

A metric of the form

$$g_{\mu\nu} = \begin{pmatrix} f_1^2 & 0 \\ 0 & f_2^2 \end{pmatrix} \tag{5.1}$$

where f_1 and f_2 are arbitrary functions, describes and system of orthogonal curvilinear coordinates in 2D. It can easily be seen that the natural tweibein is

$$e_\mu^a = \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix} \tag{5.2}$$

and a general form of the affine connection can be computed quite easily

$$\Gamma^{\kappa}_{\mu\ \nu} = \frac{1}{2} g^{\kappa\rho}\left(\frac{\partial g_{\kappa\nu}}{\partial \chi^{\mu}} + \frac{\partial g_{\kappa\mu}}{\partial \chi^{\nu}} - \frac{\partial g_{\mu\nu}}{\partial \chi^{\kappa}}\right) \tag{5.3}$$

$$= \frac{1}{f_{\kappa\kappa}^2}\left(f_{\kappa\nu}\frac{\partial f_{\kappa\nu}}{\partial \chi^{\mu}} + f_{\kappa\mu}\frac{\partial f_{\kappa\mu}}{\partial \chi^{\nu}} f_{\mu\nu}\frac{\partial f_{\mu\nu}}{\partial \chi^{\kappa}}\right) \tag{5.4}$$

$$= \begin{pmatrix} \begin{pmatrix} \frac{f_1}{f_1^2}\frac{\partial f_1}{\partial \chi^1} \\ -\frac{f_1}{f_2^2}\frac{\partial f_1}{\partial \chi^2} \end{pmatrix} & \begin{pmatrix} \frac{f_1}{f_1^2}\frac{\partial f_1}{\partial \chi^2} \\ \frac{f_2}{f_2^2}\frac{\partial f_2}{\partial \chi^1} \end{pmatrix} \\ \begin{pmatrix} \frac{f_1}{f_1^2}\frac{\partial f_1}{\partial \chi^2} \\ \frac{f_2}{f_2^2}\frac{\partial f_2}{\partial \chi^1} \end{pmatrix} & \begin{pmatrix} -\frac{f_2}{f_1^2}\frac{\partial f_2}{\partial \chi^1} \\ \frac{f_2}{f_2^2}\frac{\partial f_2}{\partial \chi^2} \end{pmatrix} \end{pmatrix} \tag{5.5}$$

The Riemann tensor is

$$R_{\rho\sigma\mu\nu} = \frac{1}{2}\left(\partial_\mu\partial_\sigma g_{\nu\rho} - \partial_\nu\partial_\sigma g_{\mu\rho} - \partial_\mu\partial_\rho g_{\nu\sigma} + \partial_\nu\partial_\rho g_{\mu\rho}\right) \tag{5.6}$$

$$- g_{\lambda\kappa}\Gamma^{\lambda}_{\mu\ \rho}\Gamma^{\kappa}_{\nu\ \sigma} + g_{\lambda\kappa}\Gamma^{\lambda}_{\nu\ \rho}\Gamma^{\kappa}_{\mu\ \sigma} \tag{5.7}$$

$$\tag{5.8}$$

and the number of independent components it can have are restricted by the Bianchi identities

$$R_{\rho\sigma\mu\nu} = -R_{\sigma\rho\mu\nu} = -R_{\rho\sigma\nu\mu} = R_{\sigma\rho\nu\mu} \tag{5.9}$$

$$R_{\rho\sigma\mu\nu} = R_{\mu\nu\rho\sigma} \tag{5.10}$$

$$R_{\rho\sigma\mu\nu} + R_{\rho\nu\sigma\mu} + R_{\rho\mu\nu\sigma} = 0 \tag{5.11}$$

$$\nabla_\kappa R_{\rho\sigma\mu\nu} + \nabla_\nu R_{\rho\sigma\kappa\mu} + \nabla_\mu R_{\rho\sigma\nu\kappa} = 0 \tag{5.12}$$

In n dimensions the number of independent components of the Riemann tensor is

$$\frac{n^2\left(n^2-1\right)}{12} \tag{5.13}$$

so in two dimensions we have only one independent component and $R_{\rho\sigma\mu\nu}$ takes the form

$$R_{\rho\sigma\mu\nu} = \begin{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & -\alpha \\ \alpha & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix} \tag{5.14}$$

To find the form of the full tensor in terms of the arbitrary functions f_1 and f_2, we need only computer one component

$$\alpha = R_{1212} \tag{5.15}$$
$$= -\frac{1}{2}\left(\partial_2^2 g_{11} + \partial_1^2 g_{22}\right) + g_{\kappa\kappa}(\Gamma^{\kappa}_{2\,1}\Gamma^{\kappa}_{1\,2} - \Gamma^{\kappa}_{1\,1}\Gamma^{\kappa}_{2\,2}) \tag{5.16}$$
$$= -\frac{1}{2}\left(\partial_2^2 f_1^2 + \partial_1^2 f_2^2\right) + f_{11}^2\left(\frac{f_1}{f_1^2}\frac{f_1}{f_1^2}\partial_2 f_1 \partial_2 f_1 + \frac{f_1}{f_1^2}\frac{f_2}{f_1^2}\partial_1 f_1 \partial_1 f_2\right) \tag{5.17}$$
$$+ f_2^2\left(\frac{f_2}{f_2^2}\frac{f_2}{f_2^2}\partial_1 f_2 \partial_1 f_2 + \frac{f_2}{f_2^2}\frac{f_1}{f_2^2}\partial_2 f_1 \partial_2 f_2\right) \tag{5.18}$$
$$= -\frac{1}{2}\left(\partial_2^2 f_1^2 + \partial_1^2 f_2^2\right) + (\partial_2 f_1)^2 + \frac{f_2}{f_1}\partial_1 f_1 \partial_1 f_2 \tag{5.19}$$
$$+ (\partial_1 f_2)^2 + \frac{f_1}{f_2}\partial_2 f_1 \partial_2 f_2 \tag{5.20}$$
$$= -f_1 \partial_2^2 f_1 - f_2 \partial_1^2 f_2 + \frac{f_2}{f_1}\partial_1 f_1 \partial_1 f_2 + \frac{f_1}{f_2}\partial_2 f_1 \partial_2 f_2 \tag{5.21}$$

and the Ricci tensor and curvature scalar are

$$R_{\sigma\nu} = g^{\rho\mu}R_{\rho\sigma\mu\nu} = g^{11}R_{1\sigma 1\nu} + g^{2}R_{2\sigma 2\nu} \tag{5.22}$$
$$R_{11} = g^{11}R_{1111} + g^{22}R_{2121} = g^{22}\alpha \tag{5.23}$$
$$R_{22} = g^{11}R_{1212} + g^{22}R_{2222} = g^{11}\alpha \tag{5.24}$$
$$R = g^{\sigma\nu}R_{\sigma\nu} = g^{11}g^{22}\alpha + g^{11}g^{22}\alpha = \frac{2\alpha}{g} \tag{5.25}$$

5.1.2 The pseudomagnetic gauge field

The spin connection

$$\omega_{\mu\ b}^{\ a} = e_{\nu}^{a} e_{\nu}^{\lambda}\Gamma^{\nu}_{\mu\,\lambda} - e_{b}^{\lambda}\partial_{\mu} e_{\lambda}^{a} \tag{5.26}$$
$$\omega_{\mu\ 1}^{\ 1} = \omega_{\mu\ 2}^{\ 2} = 0 \tag{5.27}$$
$$\omega_{\mu\ 2}^{\ 1} = e_1^1 e_2^2 \Gamma^{1}_{\mu\,2} - e_2^2 \partial_{\mu} e_1^1 \tag{5.28}$$
$$\omega_{\mu\ 1}^{\ 2} = e_2^2 e_1^1 \Gamma^{2}_{\mu\,1} - e_1^1 \partial_{\mu} e_2^2 \tag{5.29}$$
$$\omega_{\mu\ b}^{\ a} = \begin{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{f2}\partial_2 f_1 \end{pmatrix} & \begin{pmatrix} -\frac{1}{f2}\partial_2 f_1 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 \\ -\frac{1}{f1}\partial_1 f_2 \end{pmatrix} & \begin{pmatrix} \frac{1}{f1}\partial_1 f_2 \\ 0 \end{pmatrix} \end{pmatrix} \tag{5.30}$$

The Dirac matrices satisfy the commutation relations

$$[\gamma^i, \gamma^j] = 2i\varepsilon_{ijk}\gamma^k \tag{5.31}$$

and we form the antisymmetric matrix

$$\Sigma^{ab} = [\gamma^a, \gamma^b] = \begin{pmatrix} 0 & 2i\sigma_z \\ -2i\sigma_z & 0 \end{pmatrix} \tag{5.32}$$

The spin covariant derivative is defined as $\partial_\mu \to D_\mu = \partial_\mu + \Omega_\mu$ where

$$\Omega_\mu = \frac{1}{8}\omega_{\mu ab}\Sigma^{ab} \tag{5.33}$$

$$= \frac{i}{2}\sigma_z\left(\omega_{\mu 12} - \omega_{\mu 21}\right) \tag{5.34}$$

$$\Omega_1 = \frac{i}{2}\sigma_z\frac{1}{f_2}\partial_2 f_1 \tag{5.35}$$

$$\Omega_2 = -\frac{i}{2}\sigma_z\frac{1}{f_1}\partial_1 f_2 \tag{5.36}$$

From which we construct a general form of the Dirac equation in orthogonal curvilinear coordinates

$$-i\hat{\nabla}\psi = -i\hat{\gamma}^\mu D_\mu \psi \tag{5.37}$$

$$= -i\left(\frac{\gamma^1}{f1}\left(\partial_1 + \frac{i\sigma_z}{2f_2}\partial_2 f_1\right) + \frac{\gamma^2}{f2}\left(\partial_2 - \frac{i\sigma_z}{2f_1}\partial_1 f_2\right)\right)\psi = 0 \tag{5.38}$$

This equation has extra terms as a result of the spin connection when compared its flat space counterpart. By comparison with the minimal coupling to an electromagnetic potential

$$\partial_\mu \to \partial_\mu + \frac{ie}{\hbar c}A_\mu \tag{5.39}$$

These extra terms can be thought of as a gauge field coupled to the generator $\frac{\sigma_z}{2}$

$$A_\mu = \frac{\hbar c}{e}\frac{1}{\sqrt{g}}\begin{pmatrix}\partial_2 f_1 & -\partial_1 f_2\end{pmatrix} \tag{5.40}$$

The generalised curl in arbitrary coordinates is[22]

$$\nabla \times A = \frac{1}{f_1 f_2 f_3} \begin{vmatrix} \hat{e}_1 & \hat{e}_2 & \hat{e}_3 \\ \partial_1 & \partial_2 & \partial_3 \\ f_1 A_1 & f_2 A_2 & f_3 A_3 \end{vmatrix} \tag{5.41}$$

To take the curl of the vector potential and find the magnetic field, we acknowledge the existence of a three dimensional space within which the 2-manifold is embedded. The third basis vector is defined as being the unit vector perpendicular to the other two, and the manifold itself, at any point. Since motion is restricted to a 2-manifold embedded in this 3D space, we demand that all derivatives with respect to the third coordinate are zero

$$\begin{aligned}
B = \nabla \times A &= \frac{\hbar c}{e} \frac{1}{\sqrt{g}} \begin{vmatrix} \hat{e}_1 & \hat{e}_2 & \hat{e}_3 \\ \partial_1 & \partial_2 & 0 \\ f_1 \frac{1}{\sqrt{g}} \partial_2 f_1 & -f_2 \frac{1}{\sqrt{g}} \partial_1 f_2 & 0 \end{vmatrix} && (5.42) \\
&= \frac{\hbar c}{e} \frac{1}{\sqrt{g}} \left(-\partial_1 \left(\frac{1}{f_2} \partial_2 f_1 \right) - \partial_2 \left(\frac{1}{f_1} \partial_1 f_2 \right) \right) \hat{e}_3 && (5.43) \\
&= \frac{\hbar c}{e} \frac{1}{\sqrt{g}} \left(\frac{1}{f_2} \partial_2^2 f_1 + \frac{1}{f_1} \partial_1^2 f_2 - \frac{1}{f_1^2} \partial_1 f_1 \partial_1 f_2 - \frac{1}{f_2^2} \partial_2 f_1 \partial_2 f_2 \right) \hat{e}_3 && (5.44) \\
&= \frac{\hbar c}{e} \frac{1}{g} \left(f_1 \partial_2^2 f_1 + f_2 \partial_1^2 f_2 - \frac{f_2}{f_1} \partial_1 f_1 \partial_1 f_2 - \frac{f_1}{f_2} \partial_2 f_1 \partial_2 f_2 \right) \hat{e}_3 && (5.45) \\
&= -\frac{\hbar c}{e} \frac{\alpha}{g} \hat{e}_3 = -\frac{\hbar c}{2e} R \hat{e}_3 && (5.46)
\end{aligned}$$

Thus a Dirac field on a curved 2-manifold experiences a force as a result of the curvature, and this arises in the form of a magnetic field whose strength is $\frac{\hbar c}{2e}$ times the scalar curvature, oriented normal to the manifold. The force felt by a particle due to this field it always in the plane of the manifold, and perpendicular to the direction of motion, so the field does no work.

5.1.3 Examples

This relationship can be demonstrated for the two example systems from previous chapters.

In the case of the plane with cylindrically symmetric distortions, the Dirac equation is

$$-i \left[\frac{1}{\sqrt{1+f'^2}} \sigma_x \partial_r + \frac{1}{r} \sigma_y \left(\partial_\theta - \frac{i\sigma_z}{2\sqrt{1+f'^2}} \right) \right] \psi = 0 \tag{5.47}$$

and the extra gauge field is

$$\frac{ie}{\hbar c}A_\theta = -i\frac{1}{r\sqrt{1+f'^2}} \tag{5.48}$$

$$A_\mu = \begin{pmatrix} 0 & \frac{\hbar c}{e}\frac{1}{r}\frac{1}{\sqrt{1+f'^2}} & 0 \end{pmatrix} \tag{5.49}$$

We can take the curl of this field as

$$\nabla \times A = \frac{1}{r\sqrt{1+f'^2}} \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{n} \\ \partial_r & \partial_\theta & 0 \\ 0 & rA_\theta & 0 \end{vmatrix} \tag{5.50}$$

$$= \frac{1}{r\sqrt{1+f'^2}}\partial_r\left(\frac{\hbar c}{e}\frac{1}{\sqrt{1+f'^2}}\right)\hat{n} \tag{5.51}$$

so the pseudomagnetic field associated with this potential is

$$B = \nabla \times A = \frac{\hbar c}{2e}\frac{2f'f''}{r\left(1+f'^2\right)^2}\hat{z} = \frac{\hbar c}{2e}R\hat{n} \tag{5.52}$$

And in the case of the 2-sphere the Dirac equation is

$$-i\left[\frac{1}{r}\sigma_x\partial_\theta + \frac{1}{r\sin(\theta)}\sigma_y\left(\partial_\phi - \frac{i\sigma_z}{2}\cos(\theta)\right)\right]\psi = 0 \tag{5.53}$$

and the additional vector potential is

$$A_\mu = \begin{pmatrix} 0 & 0 & -\frac{\hbar c}{e}\frac{1}{r}\cot(\theta) \end{pmatrix} \tag{5.54}$$

The curl is

$$\nabla \times A = \frac{1}{r^2\sin(\theta)} \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\phi} \\ \partial_r & \partial_\theta & \partial_\phi \\ 0 & 0 & r\sin(\theta)A_\phi \end{vmatrix} \tag{5.55}$$

$$= \frac{1}{r^2\sin(\theta)}\partial_\theta\left(-\frac{\hbar c}{e}\cos(\theta)\right)\hat{r} \tag{5.56}$$

so the pseudomagnetic field associated with this potential is

$$B = \nabla \times A = \frac{\hbar c}{2e}\frac{2}{r^2}\hat{r} = \frac{\hbar c}{2e}R\hat{r} \tag{5.57}$$

This is a field normal to the surface of the sphere at any point and with constant magnitude.

5.1.4 The restricted third dimension

We can follow the same process while treating the manifold as a subspace of a three dimensional world throughout, by considering the case

$$g_{\bar{\mu}\nu} = \begin{pmatrix} f_1^2 & 0 & 0 \\ 0 & f_2^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \mathbf{g} & 0 \\ 0 & 1 \end{pmatrix} \tag{5.58}$$

$$e_{\bar{\mu}}^{a} = \begin{pmatrix} f_1 & 0 & 0 \\ 0 & f_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \mathbf{e} & 0 \\ 0 & 1 \end{pmatrix} \tag{5.59}$$

It then easily follows that

$$\bar{R} = R \tag{5.60}$$

$$\bar{\Omega_1} = \begin{pmatrix} \Omega_1 & 0 \\ 0 & 0 \end{pmatrix} \tag{5.61}$$

$$\bar{\Omega_2} = \begin{pmatrix} \Omega_2 & 0 \\ 0 & 0 \end{pmatrix} \tag{5.62}$$

$$\bar{\Omega_3} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{5.63}$$

$$\bar{A_\mu} = \frac{\hbar c}{e}\frac{1}{\sqrt{g}}\begin{pmatrix} \partial_2 f_1 & -\partial_1 f_2 & 0 \end{pmatrix} = \begin{pmatrix} A_\mu & 0 \end{pmatrix} \tag{5.64}$$

$$\bar{B} = \hat{\nabla} \times \hat{A} == \frac{\hbar c}{e}\frac{1}{\sqrt{g}}\begin{vmatrix} \hat{e_1} & \hat{e_2} & \hat{e_3} \\ \partial_1 & \partial_2 & 0 \\ f_1\frac{1}{\sqrt{g}}\partial_2 f_1 & -f_2\frac{1}{\sqrt{g}}\partial_1 f_2 & 0 \end{vmatrix} \tag{5.65}$$

$$= B = -\frac{\hbar c}{e}\frac{\alpha}{g}\hat{e}_3 = -\frac{\hbar c}{2e}\bar{R}\hat{e}_3 \tag{5.66}$$

and the result is the same.

5.2 Hints of a Further Relationship

Though extremely laborious to work through by hand, we can consider the case

$$g_{\mu\nu} = \begin{pmatrix} f_1^2 & 0 & 0 \\ 0 & f_2^2 & 0 \\ 0 & 0 & f_3^2 \end{pmatrix} \tag{5.67}$$

To arrive at a form for the Dirac equation in three curved dimensions

$$\begin{aligned}
&i\left(\frac{\gamma^1}{f_1}\left(\partial_1 + i\sigma_3\frac{\partial_2 f_1}{2f_2} - i\sigma_2\frac{\partial_3 f_1}{2f_3}\right)\right. && (5.68)\\
&+\frac{\gamma^2}{f_2}\left(\partial_2 + i\sigma_1\frac{\partial_3 f_2}{2f_3} - i\sigma_3\frac{\partial_1 f_2}{2f_1}\right) && (5.69)\\
&\left.+\frac{\gamma^3}{f_3}\left(\partial_3 + i\sigma_2\frac{\partial_1 f_3}{2f_1} - i\sigma_1\frac{\partial_2 f_3}{2f_2}\right)\right)\psi = 0 && (5.70)
\end{aligned}$$

This can be made sense of if we suppose we are seeing three gauge fields with the symmetry group SU(2); one associated with each of the spin-$\frac{1}{2}$ rotation generators, similar to the eight gauge fields in quantum chromodynamics

$$\begin{aligned}
\partial_\mu \rightarrow& \partial_\mu + \frac{i}{2}\sigma_1 A_\mu^1 + \frac{i}{2}\sigma_2 A_\mu^2 + \frac{i}{2}\sigma_3 A_\mu^3 && (5.71)\\
=& \partial_\mu + \frac{i}{2}A_\mu^i \sigma_i && (5.72)\\
A_\mu^1 =& \frac{\hbar c}{e}\frac{f_1}{\sqrt{g}}\begin{pmatrix} 0 & \partial_3 f_2 & -\partial_2 f_3 \end{pmatrix} && (5.73)\\
A_\mu^2 =& \frac{\hbar c}{e}\frac{f_2}{\sqrt{g}}\begin{pmatrix} -\partial_3 f_1 & 0 & \partial_1 f_3 \end{pmatrix} && (5.74)\\
A_\mu^3 =& \frac{\hbar c}{e}\frac{f_3}{\sqrt{g}}\begin{pmatrix} \partial_2 f_1 & -\partial_1 f_2 & 0 \end{pmatrix} && (5.75)
\end{aligned}$$

Chapter 6

Conclusions

The electronic excitations in graphene give rise to charge-carrying quasiparticles that can be described by the Dirac equation in curved space. This has been demonstrated for two types of systems: graphene monolayers with out-of-plane distortions and a carbon 2-sphere. From a coordinate based description of the shape of the manifold the Dirac equation governing the electronic properties of the system can be computed.

For systems that can be related to flat graphene through a perturbing potential, the Dirac equation can be solved by the Green's function method to find a distortion of the dispersion in response to curvature. Other graphene systems that are topologically inequivalent to a graphene monolayer are fundamentally different in their behaviour. In the case of the carbon 2-sphere the energy and momentum eigenstates are discrete, in clear contrast with those of monolayer graphene.

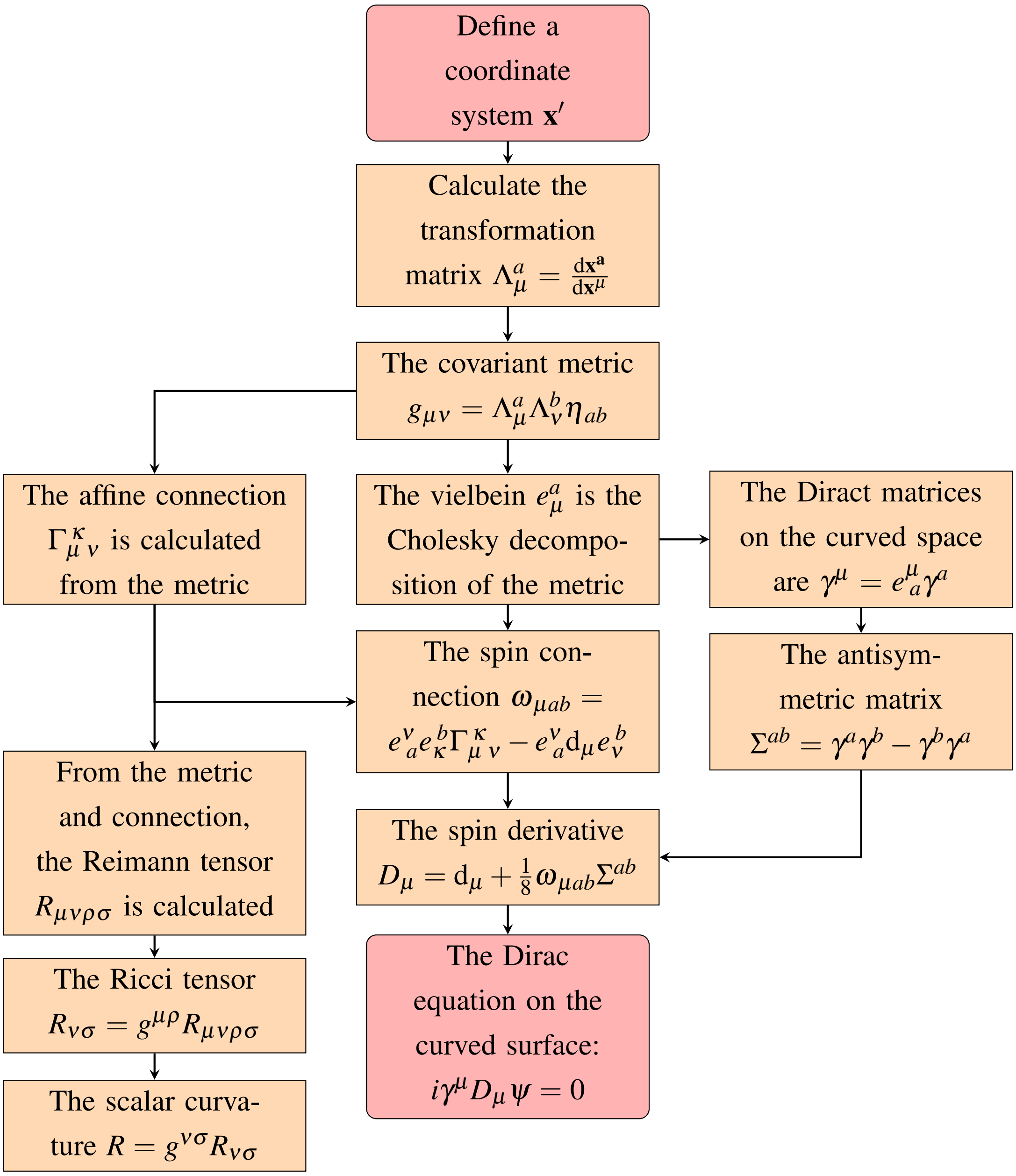
It was shown that curvature in 2D can be seen as inducing an effective pseudomagnetic field everywhere normal to the manifold, and an exact proportionality between the curvature scalar and the induced pseudomagnetic field was derived.

There is much more to be said about the remarkable properties of graphene and in particular the research potential of experimentally accessible analogue gravity in graphene devices. The possibility of a table top particle physics playground enabling the testing of theories of quantum gravity in two dimensions is an enticing one. With the recent explosion of interest and developments now rapidly being made in the analogies between different areas of physics, it may just be an analogue gravity experiment that provides the next small step towards uniting quantum theory and gravity, and the next giant leap towards understanding the universe we find ourselves part of.

I leave you with the parting thought that the seed of the next great paradigm shift could reside anywhere, with the most seemingly unrelated field of study or the most ridiclous sounding idea.

Appendix A

Mathematica Code



```
Remove["Global`*"]
Clear["Global`*"]

SetAttributes[{t, r, θ, σ, Xdim, Qdim,
  η3, μ, ν, λ, ρ, τ, κ, α, β, i, e, c, ℏ}, Constant]

$Assumptions = {Element[{t, r, θ, σ, c, ℏ}, Reals], r ≥ 0, c > 0, ℏ > 0};




(*User input*)
(*-------------------------------------------------------------*)

(*Inputs coordinates of local frame,
Qdim is number of dimensions, Q are the coordinates*)
(*Example: circular polar coordinates*)
Qdim = 3;
Q = {t, r, θ};

(*Define manifold in global lab frame,
Xdim is number of dimensions,
X are the coordinates in terms of Q*)
(*Example: Plane with cylindrically symmetric deformations f[r]*)
Xdim = 4;
X = {c * t, r * Cos[θ], r * Sin[θ], f[r]};

(*-------------------------------------------------------------*)
```

```
(*Geometric Properties*)
(*---------------------------------------------------------------*)
(*Flat metric*)
η3 = DiagonalMatrix[{1, -1, -1}];

(*Geometric Properties of Manifoldoperties*)
Λ = Transpose[Table[Dt[X[[a]], Q[[b]]], {a, 1, Xdim}, {b, 1, Qdim}]];

"Covariant Vielbein"
ecov =
 FullSimplify[CholeskyDecomposition[Λ.Transpose[Λ]], Assumptions]

"Contravariant Vielbein"
econtr = FullSimplify[Inverse[ecov]]

"Covariant Metric"
gcov = FullSimplify[
  Table[Sum[ecov[[a]][[μ]] * ecov[[b]][[ν]] * η3[[a]][[b]],
    {a, 1, Qdim}, {b, 1, Qdim}], {μ, 1, Qdim}, {ν, 1, Qdim}]]

"Contravariant Metric"
gcontr = FullSimplify[
  Table[Sum[econtr[[μ]][[a]] * econtr[[ν]][[b]] * η3[[a]][[b]],
    {a, 1, Qdim}, {b, 1, Qdim}], {μ, 1, Qdim}, {ν, 1, Qdim}]]

"Affine Connection"
Γ = Table[FullSimplify[
    Sum[1/2 * gcontr[[κ]][[λ]] * Dt[gcov[[λ]][[ν]], Q[[μ]]],
      {λ, 1, Qdim}] + Sum[1/2 * gcontr[[κ]][[λ]] *
```

```
        Dt[gcov[[λ]][[μ]], Q[[ν]]], {λ, 1, Qdim}] - Sum[1/2 *
        gcontr[[κ]][[λ]] * Dt[gcov[[μ]][[ν]], Q[[λ]]], {λ, 1, Qdim}]],
    {κ, 1, Qdim}, {μ, 1, Qdim}, {ν, 1, Qdim}];
MatrixForm[FullSimplify[%]]

(* Calculate Riemann tensor *)
Riemann =
  FullSimplify[ -Table[(Dt[Dt[gcov[[λ, ν]], {Q[[κ]]}], Q[[μ]]] +
         Dt[Dt[gcov[[μ, κ]], {Q[[λ]]}], Q[[ν]]] -
         Dt[Dt[gcov[[μ, ν]], {Q[[κ]]}], Q[[λ]]] -
         Dt[Dt[gcov[[λ, κ]], {Q[[μ]]}], Q[[ν]]]) / 2 +
      Sum[gcov[[α, β]] * Γ[[α, ν, λ]] * Γ[[β, μ, κ]], {α, 1, Qdim},
       {β, 1, Qdim}] - Sum[gcov[[α, β]] * Γ[[α, κ, λ]] * Γ[[β, μ, ν]],
       {α, 1, Qdim}, {β, 1, Qdim}], {λ, 1, Qdim},
     {μ, 1, Qdim}, {ν, 1, Qdim}, {κ, 1, Qdim}] ];

"Riemann tensor"
MatrixForm[Riemann]

(* Calculate Ricci Tensor *)
Ric = FullSimplify[
   Table[Sum[Sum[gcontr[[α, μ]] * Riemann[[α, β, μ, ν]], {α, 1, Qdim}],
     {μ, 1, Qdim}], {β, 1, Qdim}, {ν, 1, Qdim}] ];

"Ricci tensor"
MatrixForm[Ric]

"Curvature Scalar"
R = FullSimplify[
  Sum[Sum[gcontr[[ρ, σ]] * Ric[[ρ, σ]], {ρ, 1, Qdim}], {σ, 1, Qdim}]]
```

```
(*-------------------------------------------------------------*)




(*Quantum Operators*)
(*-------------------------------------------------------------*)
(*Flat Dirac matrices*)
γ = {PauliMatrix[3], ⅈ * PauliMatrix[2], -ⅈ * PauliMatrix[1]};

"Dirac matrices on Curved Surface"
γ1 = FullSimplify[
  Table[Sum[econtr[[μ, a]] γ[[a]], {a, 1, Qdim}], {μ, 1, Qdim}]];
(*/.{(ⅈ*Cos[θ]+Sin[θ])→ⅈ*Exp[-ⅈθ],
  (-ⅈ*Cos[θ]+Sin[θ])→-ⅈ*Exp[ⅈθ]}*)
MatrixForm[γ1[[1]]]
MatrixForm[γ1[[2]]]
MatrixForm[γ1[[3]]]

(*Antisymmetric Matrix*)
Σ = FullSimplify[Table[(1 / 4) * (γ[[a]].γ[[b]] - γ[[b]].γ[[a]]),
    {a, 1, Qdim}, {b, 1, Qdim}]];

(*Spin connection*)
Spinconnection =
  FullSimplify[Table[Sum[ecov[[a, ν]] * econtr[[λ, b]] * Γ[[ν, μ, λ]],
      {ν, 1, Qdim}, {λ, 1, Qdim}] -
     Sum[econtr[[λ, b]] Dt[ecov[[a, λ]], Q[[μ]]], {λ, 1, Qdim}],
    {μ, 1, Qdim}, {a, 1, Qdim}, {b, 1, Qdim}]];

(*Lower middle index of spin connection - necessary with
  (1,-1,-1) metric. Has no effect with (1,1) metric*)
```

```
Spinconnection = Table[Sum[η3[[a, b]] * Spinconnection[[μ, b, c]],
    {b, 1, Qdim}], {μ, 1, Qdim}, {a, 1, Qdim}, {c, 1, Qdim}];

"spin derivative"
Spinderivative = FullSimplify[
   Table[(1 / 2) * Sum[Spinconnection[[μ, a, b]] * Σ[[a, b]],
      {a, 1, Qdim}, {b, 1, Qdim}], {μ, 1, Qdim}]];

"Ω1"
MatrixForm[Spinderivative[[1]]]

"Ω2"
MatrixForm[Spinderivative[[2]]]

"Ω3"
MatrixForm[Spinderivative[[3]]]

(*Spin Covariant Derivative Operator*)
SpinCovD[ψ_, a_] := Dt[ψ, Q[[a]]] + Spinderivative[[a]].ψ;

(*Dirac Operator*)
Dirac[ψ_] :=
  FullSimplify[ⅈ * ℏ * Sum[γ1[[μ]].SpinCovD[ψ, μ], {μ, 1, Qdim}]];

(*Hamiltonian*)
H[ψ_] := FullSimplify[
   -ⅈ * ℏ * c * Sum[γ[[1]].γ1[[μ]].SpinCovD[ψ, μ], {μ, 2, Qdim}]];

ψ = {ψA, ψB};

"Hamiltonian acting on ψ"
MatrixForm[H[ψ]]
```

```
"Dirac Operator acting on ψ"
MatrixForm[Dirac[ψ]]

(*------------------------------------------------------------*)
```

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